LARGE REGULAR SIMPLICES CONTAINED IN A HYPERCUBE WITH A COMMON BARYCENTER

HIROKI TAMURA

Abstract. It has been shown that the n-dimensional unit hypercube contains an n-dimensional regular simplex of edge length $c\sqrt{n}$ for arbitrary $c < 1/2$ if n is sufficiently large (Maehara, Ruzsa and Tokushige, 2009). We prove the same statement holds for some $c > 1/2$ even in the special case where a regular simplex has the same barycenter as that of the unit hypercube.

1. Introduction

Let $\ell\Delta_n$ be an n-dimensional regular simplex of edge length ℓ, and let $Q_n = [-1/2, 1/2]^n$ be the n-dimensional unit hypercube. In [3], the problem of finding the largest size of an n-dimensional regular which can be contained in the unit hypercube, is considered. For a lower bound, they assert that for every $\epsilon_0 > 0$ there is an N_0 such that for every $n > N_0$ one has $((1-\epsilon_0)/2)\sqrt{n}\Delta_n \subset Q_n$. Here, "$\ell\Delta_n \subset Q_n$" means that an isometric copy of $\ell\Delta_n$ is contained in Q_n. For the upper bound, if $\ell\Delta_n \subset Q_n$, then $\ell \leq \sqrt{(n+1)/2}$, and the equality holds if and only if there exists a Hadamard matrix of order $n+1$ [5].

In this paper, we restrict the case where a regular simplex has the same barycenter as that of the unit hypercube. In this situation, the above statement for the upper bound is still valid, and moreover for a lower bound, we improve the above assertion by inductive construction from Hadamard matrices. By "$\ell\Delta_{n,0} \subset Q_n$" , we mean that an isometric copy of $\ell\Delta_n$ with barycenter at the origin is contained in Q_n. Then we have the following result.

Theorem 1. *For every n one has*

$$\left(\frac{\sqrt{336}-4-\sqrt{2}}{\sqrt{664}}\sqrt{n}\right)\Delta_{n,0} \subset Q_n.$$

Note that $(\sqrt{336}-4-\sqrt{2})/\sqrt{664} = 0.5012\cdots$, and thus this theorem improves the result of [3].

2. Proof of the main result

We denote the $n \times n$ all-one matrix by J_n, and the all-one vector of length n by $\mathbf{1}_n$. For a matrix (or a vector) $A = (a_{ij})$, we define its norm by $\|A\| = \max_{ij} |a_{ij}|$.

Let

$$f(n) := \max\{\ell \mid \ell\Delta_n \subset Q_n\}, \quad \text{and}$$
$$f_0(n) := \max\{\ell \mid \ell\Delta_{n,0} \subset Q_n\}.$$

Date: January 14, 2011.

Then we have

$$f_0(n) \le f(n) \le \sqrt{\frac{n+1}{2}}, \tag{1}$$

and $f_0(n) = \sqrt{(n+1)/2}$ holds if and only if there exists a Hadamard matrix of order $n+1$ [5].

Recall that the barycenter and the circumcenter of a regular simplex coincide, and the circumradius of Δ_n is $\sqrt{n/(2n+2)}$. From this fact, $\sqrt{2}\Delta_{n-1}$ with barycenter at the origin corresponds to an orthogonal matrix with the following form.

$$A = \begin{pmatrix} \frac{1}{\sqrt{n}} & p_1 \\ \vdots & \vdots \\ \frac{1}{\sqrt{n}} & p_n \end{pmatrix},$$

where $p_1, \dots, p_n$ are the vertices of $\sqrt{2}\Delta_{n-1}$. Let $\hat{O}_n$ be the set of all $n \times n$ real orthogonal matrices with the first column $(1/\sqrt{n})\mathbf{1}_n^T$. We denote by A_1 the matrix obtained by deleting the first column of $A \in \hat{O}_n$. Then we have

$$\hat{O}_n = \{(\frac{1}{\sqrt{n}}\mathbf{1}_n^T \; P) \mid \text{row vectors of } \frac{1}{\sqrt{2}}P \text{ are the vertices of } \Delta_{n-1,0}\},$$

and $\|A\| = \|A_1\|$ holds for $A \in \hat{O}_n$. Thus we have the following.

Lemma 2.

$$f_0(n-1) = \frac{1}{\sqrt{2}} \max_{A \in \hat{O}_n} \frac{1}{\|A\|}.$$

Proof.

$$\begin{aligned} f_0(n-1) &= \max\{\ell \mid \ell\Delta_{n-1,0} \subset Q_{n-1}\} \\ &= \max_{A \in \hat{O}_n} \max\{\ell \mid \|\frac{\ell}{\sqrt{2}}A_1\| \le \frac{1}{2}\} \\ &= \max_{A \in \hat{O}_n} \frac{1}{\sqrt{2}\|A_1\|} = \frac{1}{\sqrt{2}} \max_{A \in \hat{O}_n} \frac{1}{\|A\|}. \end{aligned}$$

□

Lemma 3. *Let*

$$A = \begin{cases} \sqrt{\frac{2}{n}} \begin{pmatrix} \frac{1}{\sqrt{2}}\mathbf{1}_n^T & \frac{1}{\sqrt{2}}v^T & C & S \end{pmatrix} & (n\text{: even}), \\ \sqrt{\frac{2}{n}} \begin{pmatrix} \frac{1}{\sqrt{2}}\mathbf{1}_n^T & C & S \end{pmatrix} & (n\text{: odd}), \end{cases}$$

where $C = (c_{ij})$ and $S = (s_{ij})$ are $n \times \lfloor (n-1)/2 \rfloor$ matrices with $c_{ij} = \cos(\theta_j + 2ij\pi/n)$ and $s_{ij} = \sin(\theta_j + 2ij\pi/n)$ respectively, and $v = (v_i)$ is the vector of length n with $v_i = (-1)^i$. Then $A \in \hat{O}_n$ for arbitrary θ_j's.

Proof. Follows from direct calculation of A^TA. □

Remark 4. Let T be a non-empty subset of $\{1, \dots, \lfloor (n-1)/2 \rfloor\}$, and let W be the submatrix of the above A consisting of the kth column of $\sqrt{2/n}C$ and the kth column of $\sqrt{2/n}S$ for $k \in T$, If n is even, let W' be the matrix W with the column $\sqrt{1/n}v^T$ adjoined. Then the set of row vectors of W (resp. W') form a spherical 2-design in $\mathbb{R}^{2|T|}$ (resp. $\mathbb{R}^{2|T|+1}$). The matrices W and W' in the special case where $\theta_j = 0$ for all j, appeared as a construction of spherical 2-designs in [4].

Proposition 5. *For every n, we have $f_0(n) \geq \sqrt{n+1}/2$.*

Proof. The matrix A given in Lemma 3 satisfies $\|A\| \leq \sqrt{2/n}$. Then Lemma 2 implies $f_0(n-1) \geq \sqrt{n}/2$. $\square$

Remark 6. The lower bound in Proposition 5 is already better than that of [3], and it can be slightly improved by choosing a matrix $A \in \hat{O}_n$ carefully. Indeed, $\|A\|$ is minimized when we set

$$\theta_j = \begin{cases} \pi/n & (n \equiv 0 \pmod 4) \\ \pi/4 & (\text{otherwise}) \end{cases}$$

for all j, and thus

$$f_0(n-1) \geq \begin{cases} \dfrac{\sqrt{n}}{2\cos(\pi/n)} & (n \equiv 0 \pmod 4) \\ \dfrac{\sqrt{n}}{2\cos(\pi/2n)} & (n \equiv 2 \pmod 4) \\ \dfrac{\sqrt{n}}{2\cos(\pi/4n)} & (\text{otherwise}). \end{cases}$$

To improve the lower bound more for large n, we use inductive construction of orthogonal matrices from Hadamard matrices.

Lemma 7. *Suppose that $A \in \hat{O}_{n+1}$ has a form*

$$A = \begin{pmatrix} \frac{1}{\sqrt{n+1}} & a & u \\ \vdots & v^T & X \\ \frac{1}{\sqrt{n+1}} & & \end{pmatrix}.$$

Then

$$\widetilde{A} = \begin{pmatrix} \frac{1}{\sqrt{n}} & \\ \vdots & X + (\sqrt{\frac{n}{n+1}} + a)^{-1}(-v^T + \frac{1}{\sqrt{n(n+1)}}\mathbf{1}_n^T)u \\ \frac{1}{\sqrt{n}} & \end{pmatrix} \in \hat{O}_n.$$

Proof. Since $AA^T = I_{n+1}$, we have

$$a^2 + |u|^2 = \frac{n}{n+1},$$
$$av + uX^T = -\frac{1}{n+1}\mathbf{1}_n,$$
$$v^T v + XX^T = I_n - \frac{1}{n+1}J_n,$$

and thus we have $\widetilde{A}\widetilde{A}^T = I_n$ by direct calculation. $\square$

From the above lemmas, we have the following.

Proposition 8. (i) $f_0(2n+1) \geq \sqrt{2} f_0(n)$,
(ii) $f_0(n-1) > f_0(n) - 1/\sqrt{2}$.

Proof. (i) Let $B_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$. If $A \in \hat{O}_n$, then $B_2 \otimes A \in \hat{O}_{2n}$ and $\|B_2 \otimes A\| = \|A\|/\sqrt{2}$. The result follows from Lemma 2.

(ii) Let A and $\widetilde{A}$ be as in Lemma 7. By a suitable change of the sign of the second column of A, we can assume $a \geq 0$. Since

$$\begin{aligned}
\|\widetilde{A}\| &= \|X + (\sqrt{\frac{n}{n+1}} + a)^{-1}(-v^T + \frac{1}{\sqrt{n(n+1)}}\mathbf{1}_n^T)u\| \\
&\leq \|A\| + \sqrt{\frac{n+1}{n}}(\|A\| + \frac{1}{\sqrt{n(n+1)}})\|A\| \\
&= \|A\|(\frac{n+1}{n} + \sqrt{\frac{n+1}{n}}\|A\|),
\end{aligned}$$

and $\|A\| \geq 1/\sqrt{n+1}$, we have

$$\begin{aligned}
&\|\widetilde{A}\|^{-1} - \|A\|^{-1} + 1 \\
&\geq \frac{1}{\|A\|(\frac{n+1}{n} + \sqrt{\frac{n+1}{n}}\|A\|)} - \frac{1}{\|A\|} + 1 \\
&= \frac{-\frac{1}{\sqrt{n(n+1)}} + (\sqrt{\frac{n+1}{n}} - 1)\|A\| + \|A\|^2}{\|A\|(\sqrt{\frac{n+1}{n}} + \|A\|)} \\
&= \frac{(-\frac{1}{\sqrt{n+1}} + \|A\|)(\frac{1}{\sqrt{n}} + \|A\|) + (\sqrt{\frac{n+1}{n}} - 1)(1 - \frac{1}{\sqrt{n+1}})\|A\|}{\|A\|(\sqrt{\frac{n+1}{n}} + \|A\|)} \\
&> 0,
\end{aligned}$$

and thus the result follows from Lemma 2. □

Theorem 9. *Let $k \geq 1$. If there exists a Hadamard matrix of order $n+k$, we have*

$$f_0(n) \geq \frac{\sqrt{n+k} - k + 1}{\sqrt{2}},$$

and equality holds if and only if $k = 1$. In particular, if there exists a Hadamard matrix of order $4m$ for any $m \leq M$, then $f_0(n) > (\sqrt{n+4} - 3)/\sqrt{2}$ holds for any $n \leq 4M - 1$.

Proof. The former statement is a direct consequence of Proposition 8 (ii). Since $\sqrt{n+k} - k + 1$ is decreasing on k, the latter statement follows. □

If the Hadamard conjecture is true, we have $f_0(n) > (\sqrt{n+4} - 3)/\sqrt{2}$ for any n. This lower bound is close to the upper bound (1) if n is sufficiently large. Even if we do not assume the Hadamard conjecture, we can estimate a lower bound of $f_0(n)$ by Proposition 8.

Lemma 10. *Let N be a positive integer. If $f_0(n) \geq c\sqrt{n/2}$ holds for any n with $N \leq n \leq 2N - 1$, then $f_0(n) > (c - (1 + \sqrt{2})/\sqrt{N})\sqrt{n/2}$ for any $n \geq N$.*

Proof. First, we show that

$$f_0(n) \geq c\sqrt{\frac{n}{2}} - \frac{\sqrt{2}^k - 1}{2 - \sqrt{2}} \tag{2}$$

holds for any n and k with $2^k N \le n \le 2^{k+1}N - 1$, $k \in \mathbb{Z}_{\ge 0}$. If (2) holds for some n and k, then by Proposition 8, we have

$$f_0(2n) > \sqrt{2} f_0(n) - \frac{1}{\sqrt{2}} \ge c\sqrt{n} - \frac{\sqrt{2}^{k+1} - 1}{2 - \sqrt{2}}$$

and

$$\begin{aligned} f_0(2n+1) = \sqrt{2} f_0(n) &\ge c\sqrt{n} - \frac{\sqrt{2}^{k+1} - \sqrt{2}}{2 - \sqrt{2}} \\ &= c\sqrt{\frac{2n+1}{2}} - \frac{\sqrt{2}^{k+1} - 1}{2 - \sqrt{2}} + c(\sqrt{n} - \sqrt{\frac{2n+1}{2}}) + \frac{1}{\sqrt{2}}. \end{aligned}$$

Since $c \le \sqrt{(n+1)/n}$ by (1), we can derive $c(\sqrt{n} - \sqrt{(2n+1)/2}) + 1/\sqrt{2} > 0$ for $n \ge 1$. Thus, by induction on k, (2) holds for any n and k with $2^k N \le n \le 2^{k+1}N - 1$, $k \in \mathbb{Z}_{\ge 0}$. Therefore

$$\begin{aligned} \sqrt{\frac{2}{n}} f_0(n) &\ge c - \frac{1}{\sqrt{n}} \frac{\sqrt{2}^k - 1}{\sqrt{2} - 1} \\ &> c - \frac{1}{\sqrt{2^k N}} \frac{\sqrt{2}^k}{\sqrt{2} - 1} \\ &= c - \frac{1 + \sqrt{2}}{\sqrt{N}}. \end{aligned}$$

□

Proof of Theorem 1. The smallest order for which no Hadamard matrix is presently known is 668 [1, 2]. Thus $f_0(n) > (\sqrt{n+4} - 3)/\sqrt{2}$ holds for any $n \le 663$ by Theorem 9. Since $(\sqrt{n+4} - 3)/\sqrt{n}$ is a increasing function, we can set $N = 332$ and $c = (\sqrt{336} - 3)/\sqrt{332}$ in Lemma 10. Then we have

$$\frac{f_0(n)}{\sqrt{n}} > \frac{c}{\sqrt{2}} - \frac{(1 + \sqrt{2})}{\sqrt{2N}} = \frac{\sqrt{336} - 4 - \sqrt{2}}{\sqrt{664}}$$

for $n \ge 332$. For $n < 332$, we have $f_0(n)/\sqrt{n} \ge \max\{\sqrt{n+1}/2\sqrt{n}, (\sqrt{n+4} - 3)/\sqrt{2n}\}$ by Proposition 5 and Theorem 9. This lower bound exceeds $(\sqrt{336} - 4 - \sqrt{2})/\sqrt{664}$. □

References

[1] R. Craigen and H. Kharaghani, Hadamard matrices and Hadamard designs, in: Handbook of Combinatorial Designs (C. J. Colbourn and J. H. Dinitz, eds.), Second Edition, pp. 273–280, Chapman & Hall/CRC Press, Boca Raton, FL, 2007.

[2] H. Kharaghani and B. Tayfeh-Rezaie, A Hadamard matrix of order 428, J. Combin. Des. 13 (2005), 435–440.

[3] H. Maehara, I. Z. Ruzsa and N. Tokushige, Large regular simplices contained in a hypercube, Period. Math. Hungarica 58 (2009), 121–126.

[4] Y. Mimura, A construction of spherical 2-design, Graphs Combin. 6 (1990), 369–372.

[5] I. J. Schoenberg, Regular simplices and quadratic forms, J. Lond. Math. Soc. 12 (1937), 48–55.

Graduate School of Information Sciences, Tohoku University, Sendai, 980-8579 Japan

E-mail address: `tamura@ims.is.tohoku.ac.jp`